

2,3,4-Trinitrotoluene  
602-29-9 | DTXSID60208944

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 4.60 days

Global applicability domain: Outside

Local applicability domain index: 2.45e-01

Confidence level: 8.78e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Propylbenzene</div> <div>Measured: 24.3</div> <div>Predicted: 4.02</div>	<div>Image not found</div> <div>1-Methyl-2-propylbenzene</div> <div>Measured: 12.5</div> <div>Predicted: 3.17</div>	<div>Image not found</div> <div>9-Ethyl-9H-fluorene</div> <div>Measured: 2330</div> <div>Predicted: N/A</div>
<div>Image not found</div> <div>5-Methylindan</div> <div>Measured: 4.93</div> <div>Predicted: 2.25</div>	<div>Image not found</div> <div>3-Ethyltoluene</div> <div>Measured: 12.5</div> <div>Predicted: 3.26</div>	